 DOI: 10.1002/mawe.200800346

Ausbreitungsverhalten mikrostrukturell kurzer Ermüdungsrisse – experimentelle Charakterisierung und mechanismenorientierte Simulation

Propagation behaviour of microstructural short fatigue cracks – experimental characterization and mechanism-based simulation

H.-J. Christ[1], O. Düber[1], H. Knobbe[1], C.-P. Fritzen[2], U. Krupp[3], B. Künkler[2], P. Köster[2]

In diesem Beitrag werden Ergebnisse eines interdisziplinären Forschungsprojekts präsentiert, welches die Autoren während der letzten sieben Jahren durchgeführt haben. Thema des Projekts war die experimentelle Charakterisierung und mechanismenbasierte Simulation mikrostrukturell kurzer Risse. Es wurden Ermüdungsexperimente an dem austenitisch-ferritischen Duplexstahl X2 CrNiMoN 22–5-3 durchgeführt. Dabei konnte gezeigt werden, dass mikrostrukturelle Eigenschaften wie Korngröße, Phasenverteilung oder lokale Fließspannung des Korns, in welchem sich die Rissspitze befindet, den wachsenden Riss beeinflussen.

Auf Basis der experimentellen Ergebnisse wurde ein mechanismen-orientiertes Modell entwickelt, welches das Ausbreitungsverhalten kurzer Risse physikalisch begründet beschreiben kann. Mikrostrukturelle Parameter wie Körngröße, Kornverteilung, Kornorientierung usw. sind im Modell berücksichtigt, indem gemessene Werte einer virtuell erzeugten Mikrostruktur zugewiesen werden. Die Simulation findet dann in dieser virtuellen Mikrostruktur statt. Der Vergleich zwischen beobachteten und simulierten Werten zeigt eine ausgezeichnete Übereinstimmung.

Schlüsselworte: Ausbreitung kurzer Ermüdungsrisse, mikrostrukturelle Barrieren, Randelementemethode, virtuelle Mikrostruktur

This paper presents results of an interdisciplinary research project, which was undertaken by the authors during the past seven years on the subject of experimental characterization and modelling of microstructurally short fatigue crack growth. Fatigue testing was carried out on the austenitic-ferritic duplex stainless steel X2 CrNiMoN 22–5-3. It was shown clearly that microstructural features like grain size, phase distribution or yield stress of the grain containing the crack tip control an advancing short crack.

On the basis of these findings, a mechanism-oriented model was established, which is able to simulate the growth of microstructurally short fatigue cracks in a physically reasonable way. Microstructural parameters like grain size, grain distribution, grain orientation etc. are taken into account by assigning measured values to a modelled microstructure, in which the crack growth simulation takes place. The comparison of experimentally observed and calculated values shows excellent agreement.

Key words: short fatigue crack propagation, microstructural barrier, boundary element method, virtual microstructure

1 Introduction

Cyclically loaded components in structural applications often undergo a stress amplitude, which is close to the fatigue limit of the material used. Under such conditions, crack initiation and short crack propagation is considered to play an important role. It is well established that in high cycle fatigue (HCF) cracks propagate in stage I during a rather large fraction of fatigue life (up to 90 % of the number of cycles until failure, N_f). The propagation behaviour of these so-called microstructurally short fatigue cracks is strongly affected by microstructural properties, such as the grain size and the presence of phase boundaries, and cannot be described using linear-elastic fracture mechanics. Because of the significance of crack initiation and early crack propagation for cyclic life, new concepts and experimental methods have to be applied in order to provide a robust and reliable fatigue life assessment. Since a continuum-based description of the material is not adequate in the case of short cracks, no general analytical solution for this problem can be expected. In fact, a boundary element method was chosen in the framework of the study presented in this paper so that the computational effort is strongly reduced compared to finite element methods.

In a former study a titanium alloy was investigated as a first step in order to allow the determination of principle mechanisms for short crack propagation [1, 2]. In the next step, a duplex steel was used enabling the examination of phases with different properties and their influence on crack advance. The experimental results obtained on this material are presented in the following. Then the model is introduced and experimental and simulated results are compared.

1 Institut für Werkstofftechnik, Universität Siegen

2 Institut für Mechanik und Regelungstechnik, Universität Siegen

3 Fakultät Ingenieurwissenschaften und Informatik, Fachhochschule Osnabrück

2 Experimental

In order to reveal the influence of different kinds of boundaries and phases with different yield strengths on the short crack propagation, the duplex stainless steel X2 CrNiMoN 22–5-3 with a two-phase microstructure consisting of the austenitic γ phase (fcc) and the ferritic α phase (bcc) was chosen for investigation. The material was delivered in form of hot rolled and solution annealed bars (25 mm diameter) with a fine, lamellar microstructure and an austenite/ferrite-ratio of approximately 1. This condition was heat treated in order to simplify the experimental work on the effect of grain/phase boundaries on crack propagation (4h at 1250 °C, 3h 1250 °C → 1050 °C, water quenched). The annealing procedure resulted in an austenite grain size of about 33µm, a ferrite grain size of about 46µm and a volume fracture of both α and γ of ≍50 pct.

Push-pull fatigue experiments were carried out in a servo-hydraulic testing system at room temperature in laboratory atmosphere under various stress amplitudes on electrolytically polished, cylindrical specimens. The specimens were shallow-notched in order to limit the crack initiation sites to a defined area.

Crack growth was monitored by means of scanning electron microscopy. The application of electron backscatter diffraction (EBSD) in combination with suitable software (TSL OIM^{TM}) allowed to collect phase and crystallographic orientation data of large areas, providing the basis for the calculation of Schmid factors, misorientation angles and activated slip systems.

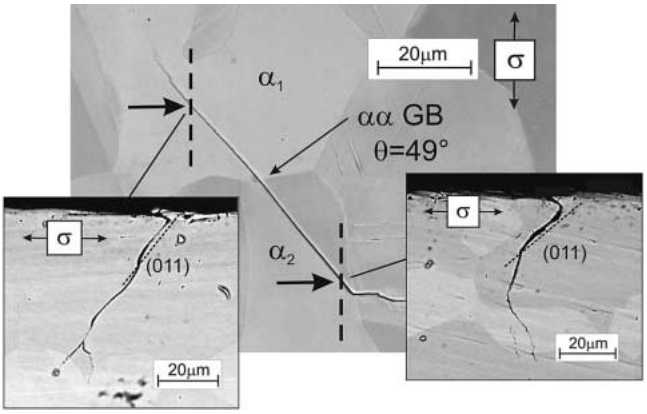

Bild 2. Risswachstum an der Oberfläche und im Inneren über eine Korngrenze mit hoher Missorientierung des Gitterwinkels.

Figure 2. Crack growth on and under the surface across a grain boundary with high lattice misorientation.

3 Results

3.1 Crack initiation

Examinations in the SEM combined with orientation measurements indicated that most of the cracks initiated near grain boundaries, though the growth frequently occurred transgranularly. It seems that the applied load induces high stresses near or at grain/phase boundaries, which is explainable by considering elastic anisotropy. Depending on the misorientation between neighbouring grains and slip compatibility at grain or phase boundaries, additional stresses develop, which contribute to the local stress state. This can be demonstrated by FEM calculations, *Figure 1*a. Here, cracks that initiated at grain or phase boundaries together with slip markings as a result of plastic deformation are shown. The results of an elastic-crystalplastic calculation are displayed in Figure 1b. This means plastic flow is permitted if the shear stress on a slip system exceeds the shear strength. Therefore slip deformation on the slip plane, which is stressed highest is displayed instead of stress. The brighter the colour is, the higher the slip deformation. Although the major crack is not indicated by high slip deformation, the occurrence of slip markings in the γ grains is reproduced. The interaction points of slip lines with grain boundaries are often the crack initiation sites.

The input parameters for the calculations are the grain shape and the crystallographic orientations. It is obvious, that anisotropy effects lead to elevated stresses, which accounts for crack initiation. Elastic anisotropy also explains, why plastic deformation frequently happens on slip systems with a much lower Schmid factor than the maximum Schmid factor in the grain.

3.2 Short crack propagation

The propagation of short cracks is also influenced by the crystallographic orientation relationship of neighbouring grains. It is known from the literature and was confirmed by the results obtained in this study that high-angle grain boundaries, which separate grains of high difference in their crystallographic orientation, hinder the spread of plastic deformation and, as a consequence, crack growth is blocked or totally stopped. In contrast, low-angle grain boundaries have only small or no effect on the crack propagation rate.

It must be pointed out that, since microstructurally short cracks grow in stage I (which means on specific glide planes), it is more precise to say that the misorientation between the glide planes in adjacent grains is the controlling parameter (as it is stated in a study by *Zhai* et al. [3]) and not the misorientation between the lattices of the grains. Experimental evidence is given in *Figure 2*. Although EBSD measurements yielded a high misorientation between the lattices of the grains α_1 and α_2, crossing of the $\alpha_1\alpha_2$-grain boundary neither leads to a significant deflection in the crack path nor to a retardation of the crack growth [4].

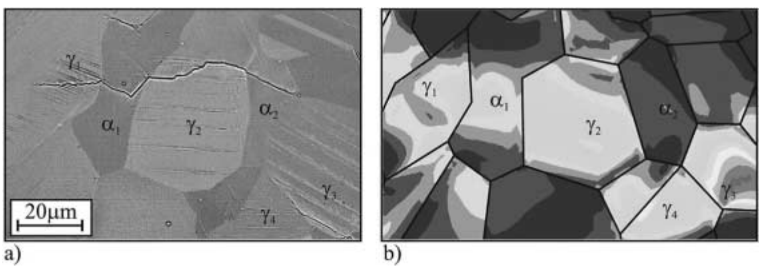

Bild 1. FEM-Berechnung des Anisotropieeffekts.
a) Risse und plastische Verformung im Duplexstahl;
b) Elastisch-plastische Berechnung des Anisotropieeffekts. Bereiche mit hoher Abgleitung sind hervorgehoben.

Figure 1. FEM-calculations of the effect of anisotropy.
a) Cracks and plastic deformation in the duplex steel;
b) Elastic-plastic calculation of anisotropy effects. Here slip deformation is highlighted.

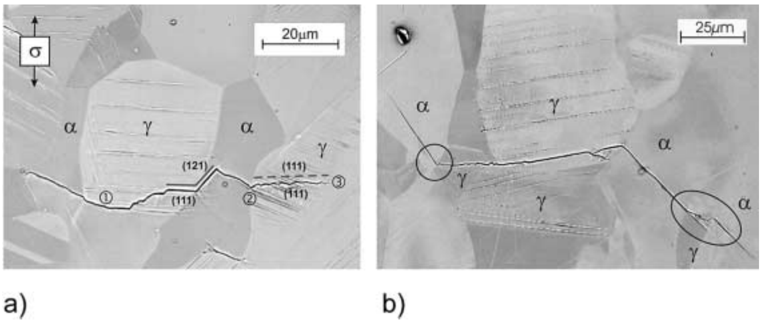

Bild 3. a) Risswachstum in Einfachgleitung (zwischen ① und ②) und Mehrfachgleitung (zwischen ② und ③); b) Änderung des Rissausbreitungsmechanismus von Mehrfachgleitung zurück zur Einfachgleitung in Abhängigkeit der lokalen Fließspannung.

Figure 3. a) Crack growth in single slip (between ① and ②) and double slip (between ② and ③); b) Change of the propagation mechanism from double slip back to single slip, depending on the local yield stress.

Since it is known from former experimental investigations on other materials [1] that underneath the specimen surface short cracks also grow in stage I on certain slip planes up to a certain depth, polishing experiments perpendicular to the specimen surface were done, in order to evaluate the crack paths in the bulk of the two grains α_1 and α_2. As can be seen in Figure 2, the crack paths in the bulk have only a small deviation of about 13° to each other. Orientation calculations showed, that in both grains the crack grew on a (011)-plane, which should have a theoretical deviation of 11° under the given grain orientations. This confirms the role of the misorientation between the slip planes.

As a consequence of the two-phase structure, the behaviour of short cracks in a material consisting of phases with different yield strengths and containing different kinds of boundaries could be examined. It turned out that under HCF conditions the phase with the higher yield stress (which is the ferritic phase in this case) activates only one slip system, which leads to crack growth in single slip. The softer austenitic phase exhibits single slip crack growth in rare cases only (for example when the crack is very short or if only one slip system is oriented favourably for plastic deformation). Most of the time the cracks grow according to a double slip mechanism. This mechanism produces a crack path perpendicular to the stress axis by alternating activation of two slip planes, similar to the Neumann description for stage II-crack growth. An example is given in *Figure 3*a. Orientation measurements of the grains involved showed that between the points ① and ② the crack grew in single slip on the slip planes indicated, whereas between the points ② and ③ crack propagation was in double slip by alternating activation of the (111) and (-111) slip plane, as could be shown by vector calculations [4].

The term „crack growth in double slip“ instead of stage II-crack growth was chosen in order to avoid confusion. The difference between crack growth in double slip and stage II-crack growth is that in double slip the crack can return to single slip crack growth, if the plastic zone at the crack tip is not able to activate the second slip plane. This can be the case when the crack enters a new grain with a different orientation and/or a higher yield stress. An example is given in Figure 3b. The circled points denote a change from double slip back to single slip. As suggested above, these changes are connected with a phase change from austenite to ferrite. In the softer austenite, more than one slip system is activated. If the crack crosses a γ/α-phase boundary and enters a harder ferrite grain, only one slip system is activated for slip deformation and crack growth, and the crack propagates in single slip. Under HCF conditions with small loading amplitudes, this can happen even at very long crack lengths. Because of this one might suggest a third stage of crack growth in addition to the established stages I and II. Stage I could be subdivided into stage Ia (the „normal“ stage I-propagation in single slip) and stage Ib (stage I-propagation in double slip with the possibility to change back to single slip). Since it is necessary to have at least two different phases with a sufficient difference in their yield stresses, such a classification seems to be reasonable only for multi-phase materials.

The results obtained on the crack growth rate led to the conclusion that crack propagation in single slip is faster than in double slip. This plays a role concerning the influence of the geometrical arrangement of the phases, as it is explained in the next paragraph.

3.3 The role of the spacial arrangement of the phases

A special feature of materials containing multiple phases with different properties is that crack growth is affected by the distribution of these phases in space. One of the reasons is the above-mentioned dependency of single slip or double slip crack growth with respect to the accordant phase. Since single slip crack growth is faster than crack growth in double slip, a phase distribution would be beneficial in terms of lifetime, where the crack spends more time in the phase that exhibits double slip. The phase distribution can be characterised by stereological parameters, whereof the most important in this context are the contiguity and the fraction of clusters. The contiguity is a measure for the connectivity of the grains of a phase, the fraction of clusters describes to what extent a phase exists as inclusion or matrix in the other phase. Such parameters can be obtained by image analysis methods on metallographic sections [5]. By using measured values for generating a modelled microstructure and executing crack growth simulations in this microstructure, the influence of the spatial arrangement on crack growth can be visualized, as is shown in a later section.

4 Modelling of short fatigue cracks

4.1 Short crack model

Based on the fatigue crack growth description of *Navarro* and *de los Rios* [6], which takes into account the role of microstructural barriers, a simulation was developed, where the crack and its plastic zone is modelled as a slip band consisting of slip band pieces stringed together. In the model, the idea of *Blomerus* and *Hills*, who stated that a tangential displacement of the slip band can be described by edge dislocations [7], is realized using „mathematical“ dislocations, which represent a displacement discontinuity. A slip band modelled with such dislocations (which are termed slip band or shear elements)

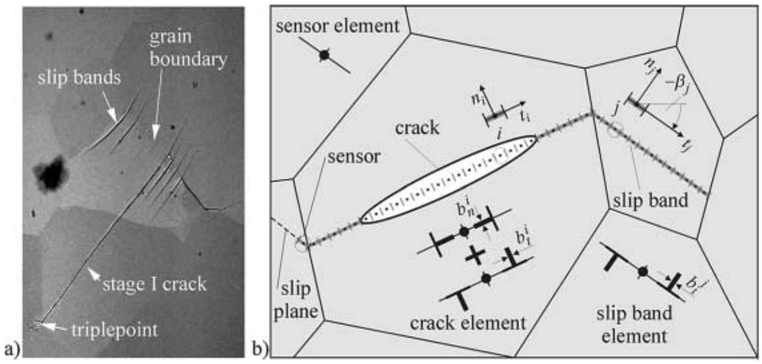

Bild 4. a) Stadium I Riss und b) Modell mit Randelementen.

Figure 4. a) Stage I crack and b) model with boundary elements.

is shown in *Figure 4*. If the shear stress on such a slip band becomes greater than the resistance of dislocations to motion, the material deforms plastically. The part of the slip band, which, in addition to the shear deformation, is allowed to open is defined as the crack. The crack is formed by crack elements, consisting of a slip band element and an additional element, which is able to perform normal displacements. So the crack with its plastic zone is represented by a dislocation distribution. The dislocations are mutually affecting each other. The influence of an element *j* on an element *i* is described by an influence function G^{ij}. Summation over all elements leads to an equation system, which together with the boundary conditions delivers a set of inequalities for the normal and shear stresses.

$$\sigma^i_{nn} = \sum_{j=1}^{p} G^{ij}_{nn,n} b^j_n + \sum_{j=1}^{p+gq} G^{ij}_{nn,t} b^j_t + \sigma^{i\infty}_{nn} \leq 0 \quad i = 1 \ldots p \tag{1}$$

$$|\tau^i_{nn}| = \left| \sum_{j=1}^{p} G^{ij}_{t,nn} b^j_n + \sum_{j=1}^{p+q} G^{ij}_{tn,n} b^j_t + \tau^{j\infty}_{tn} \right| \begin{cases} = 0 & i = 1 \ldots p \\ \leq \tau_b & i = p+1 \ldots p+q \end{cases} \tag{2}$$

$$b_n \geq 0 \quad i = 1 \ldots p \tag{3}$$

Here, *p* is the number of elements in the crack and *q* the number of activated elements (elements, where the shear stress has reached the critical shear stress) in the plastic zone. $\sigma^I_{nn}\infty$ is the global normal stress and τ^i_{tn} the resulting shear stress acting on an element *i*. Inequality (3) states that the crack faces are not able to penetrate each other and is used to model roughness-induced crack closure.

The crack propagation rate *da/dN* is calculated by a power-law function, assuming according to the model of *Navarro* and *de los Rios* that the following expression holds true:

$$\frac{da}{dN} = C \cdot \Delta CTSD^m \tag{4}$$

Here Δ*CTSD* is the range of the crack tip slide displacement, *m* is a constant similar to the exponent in the Paris-law and *C* can be regarded as a measure for the irreversibility of slip displacement. The crack tip opening displacement *CTOD* is equal to zero because the model does not allow normal displacements in the plastic zone. Equation 4 is based on the idea that plastic sliding due to external loads causes dislocation emission at the crack tip and that during reverse loading dislocations of opposite sign are emitted [8]. Hence, vacancies are produced leading to crack advance.

Due to the barrier effect of grain and phase boundaries an extension of the plastic zone into the neighbouring grain is prevented, which causes a dislocation pile up in front of the boundary. This results in a stress concentration in the neighbouring grain. In the model, the grain boundary is broken and the plastic zone expands into the next grain once a critical stress intensity is reached to activate a dislocation source on a slip system behind the barrier. Thus, the stress intensity on all available slip planes is calculated by so-called sensor elements. A more detailed description of the model can be found in [2, 5, 9].

In order to find a physical explanation for the transition from the single-slip to the double-slip mechanism, the stress state around the crack tip of a stage Ia crack was analysed. It was shown that the shear stress on inactive slip systems at the crack tip increases with growing crack length [10, 11]. Therefore the shear stress on all available slip systems is monitored in the model by means of sensor elements positioned

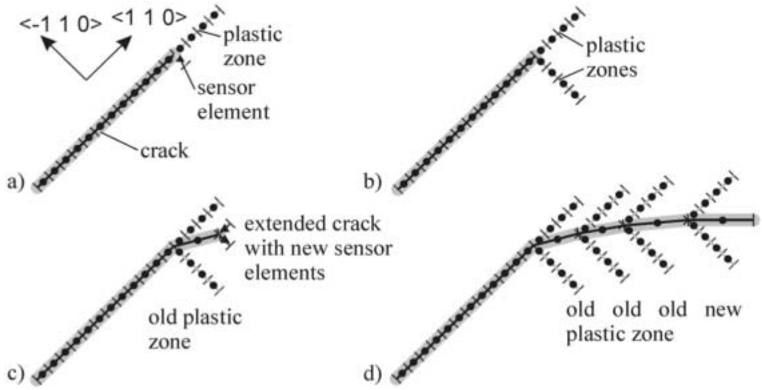

Bild 5. Übergang von Einfach- zur Mehrfachgleitung

Figure 5. Transition from the single to the double slip mechanism

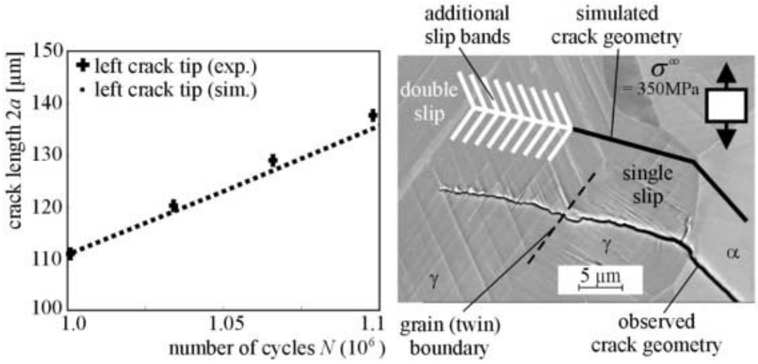

Bild 6. Simulation der Rissausbreitung in Mehrfachgleitung mit alternierender Aktivierung zweier Gleitsysteme.

Figure 6. Simulation of crack advance in double slip by alternating activation of two slip planes.

at the crack tip (*Figure 5*a). Once a critical shear stress at a sensor is reached, a second slip band is activated at the crack tip in the short crack model (Figure 5b) and the crack propagation changes from the single to the double slip mechanism. Now, plastic deformation occurs on both active slip bands, resulting in a crack growth Δa_1 on the first slip plane and a crack growth Δa_2 on the second one. Thus, the new crack tip is determined by adding these vectors to the previous crack tip (Figure 5c). Hence, with increasing crack length, the crack is deflected on a path perpendicular to the loading axis (Figure 5d).

4.2 Verification and results

In order to verify the model, the geometry of real fatigue cracks was given as an input into the simulation and the crack propagation was calculated. The comparison of the measured and calculated crack path and the propagation rate shows very good agreement, *Figure 6*. Unfortunately, the simulation could not be carried out for more cycles because the specimen broke due to the evolution of a different crack. Thereby, it should be mentioned that all parameters (also those in Eq. 4) were the same for all simulations.

In addition to the simulation of cracks with defined geometry, it is possible to simulate cracks, which find their path autonomously in a virtual single- or multiphase microstructure that is synthetically generated using the Voronoi technique [12] (*Figure 7*).

The crack starts to grow on a slip band in one grain and can propagate through several grains in the single slip mechanism. Once a critical stress in a defined distance (thus representing a stress intensity) on an additional slip plane is reached, this plane is activated and the crack growth continues in the double slip mechanism. In the double slip mechanism the crack path changes to a direction perpendicular to the external load, which is the direction of stage II-crack propagation.

By performing crack growth simulations in different virtual duplex microstructures the influence of the arrangement of phases was determined. For this purpose, a crack was placed in a microstructure representing a certain set of parameters and subjected to a calculation that reproduces cyclic loading conditions. Also, the experimentally obtained yield stresses were assigned to the phases. The results of a number of such simulations are shown in *Figure 8*. Here the relative lifetime of the respective microstructures is shown with the cor-

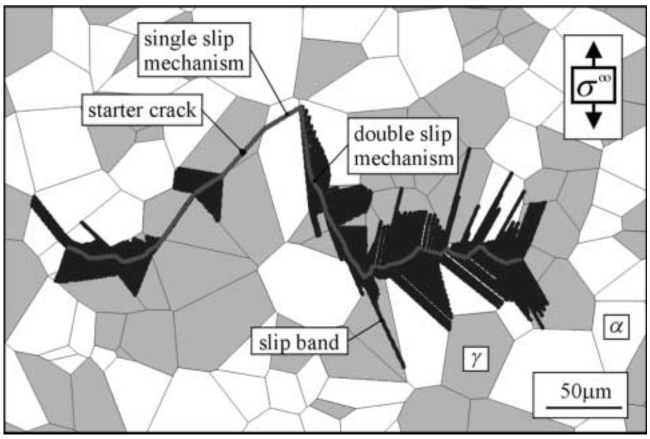

Bild 7. Simulation der Rissausbreitung in einer virtuellen Mikrostruktur.

Figure 7. Simulation of crack growth in a virtual microstructure.

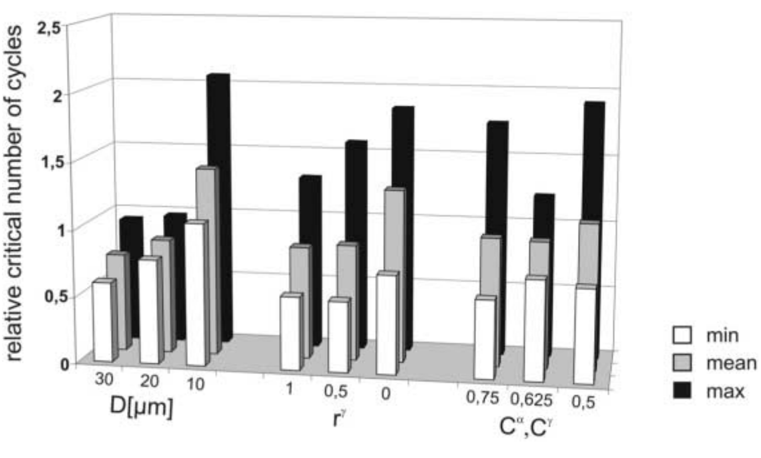

Bild 8. Abhängigkeit der Lebensdauer von mikrostrukturellen Parametern. Für jeden Parameter wurden 10 Rechnungen durchgeführt (insgesamt 90 Rechnungen). Weiß stellt die minimale Lebensdauer dar, Schwarz die maximale und Grau die mittlere. Die Ergebnisse sind auf die durchschnittliche Lebensdauer aller 30 Rechnungen für einen Parameter bezogen, welches als relative kritische Zyklenzahl bezeichnet wird.

Figure 8. The dependence of lifetime on microstructural parameters. Displayed are the results of ten simulations for each value, respectively (90 simulations in total). White is the minimal occurring lifetime, black the maximum and grey the mean value. The results are related to the mean lifetime obtained from the 30 simulations of each group varying one parameter, which yields the relative critical number of cycles.

responding geometrical parameters. Per definition the end of lifetime was reached, when the crack was 300µm long. The varied parameters are the grain size *D*, the fraction of clusters *r* and the contiguity C^{α}/C^{γ}, according to the values noted at the abscissa. It turned out that a higher grain size leads to shorter fatigue life, as expected, and that a value of r_{γ}=0 (which means that the austenite serves as the matrix phase) is beneficial for lifetime, as well as a contiguity of about 0.5 for both phases [5, 13].

5 Conclusions

By extensive experimental investigations on the initiation and propagation of microstructurally short fatigue cracks in a duplex stainless steel several features and mechanisms concerning this topic were found. The influence of the microstructure leads to a different fatigue behaviour of short cracks (in particular crack propagation) as compared to long cracks. The examination of a material containing two different phases enabled to study the effect of grains of different yield stresses, which was giving rise to different crack growth mechanisms. In this context the geometrical configuration of the phases was proven to play an important role for fatigue lifetime and a third stage of crack propagation, termed „stage Ib“, was observed.

A two-dimensional mechanism-oriented short crack model was established, which describes the propagation of stage I cracks on single slip bands. With the findings from the duplex steel, the model was enhanced in such a way that double slip crack propagation and the transition from single slip to double slip mechanism can be simulated. A comparison between the computed crack propagation and the growth of experimentally observed fatigue cracks shows an excellent agreement. The model can be used to simulate the crack growth in virtual microstructures allowing the analysis of the effect of microstructure on fatigue life. The information can be use as a basis for an optimization of a real material with respect to fatigue performance.

6 Acknowledgement

The authors would like to express their sincere gratitude to Deutsche Forschungsgemeinschaft for financial support without which the study would not have been possible.

7 References

1. W. Floer, Ph.D. Thesis, Universität Siegen, Germany, **2003**.
2. A. Schick, Ph.D. Thesis, Universität Siegen, Germany, **2004**.
3. T. Zhai, A. J. Wilkinson, J. W. Martin, *Acta Mat.* **2000**, *48*, 4917.
4. O. Düber, B. Künkler, U. Krupp, H.-J. Christ, C.-P. Fritzen, *Int. J. of Fatigue* **2006**, *28*, 983.
5. O. Düber, B. Künkler, U. Krupp, H.-J. Christ, C.-P. Fritzen, *Pract. Metall.* **2006**, *XLIII*, 88.
6. A. Navarro, E. R. de los Rios, *Phil. Mag. A* **1988**, *57*, 15.
7. P. M. Blomerus, D. A. Hills, *J. of Strain Analysis* **1998**, *33*, 315.
8. A. J. Wilkinson, S. G. Roberts, *Script. Mat.* **1996**, *35*, 1365.
9. U. Krupp, Fatigue crack propagation in metals and alloys, Wiley-VCH, Weinheim New York **2007**.
10. B. Künkler, O. Düber, P. Köster, U. Krupp, C.-P. Fritzen, H.-J. Christ, *Eng. Frac. Mech.* **2008**, *75*, 715.
11. B. Künkler, Ph.D. Thesis, Universität Siegen, Germany, **2007**.
12. G. F. Voronoi, *Z. für Reine und Angew. Math.* **1908**, *134*, 198.
13. B. Künkler, A. Schick, C.-P. Fritzen, W. Floer, U. Krupp, H.-J. Christ, *Steel Research* **2003**, *74*, 514.

Korrespondenzautor: H.-J. Christ, Institut für Werkstofftechnik, Universität Siegen, D-57068 Siegen, Germany, E-mail: hans-juergen.christ@uni-siegen.de

Eingegangen in endgültiger Form: 28. Juli 2008 T 346